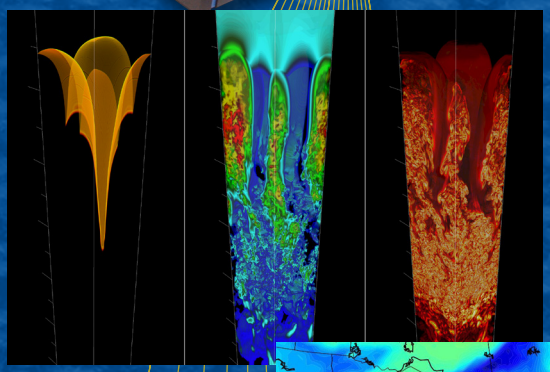
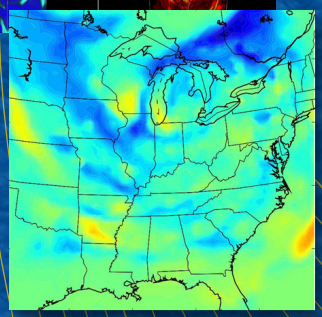
Argonne NATIONAL LABORATORY

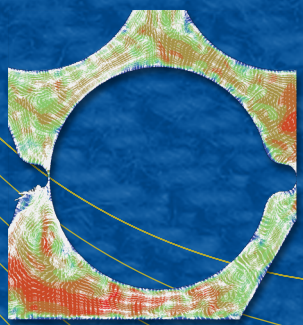
# Gateway for Scientific Discovery

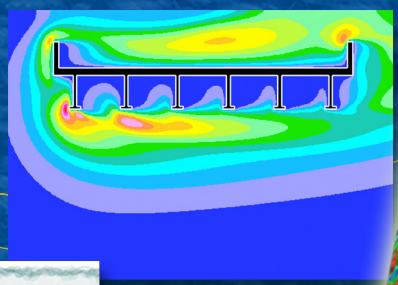
## ARGONNE LEADERSHIP COMPUTING FACILITY

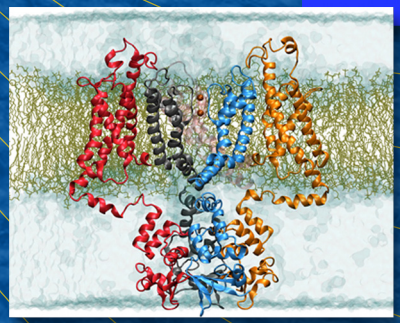
Dedicated to Breakthrough Science and Engineering

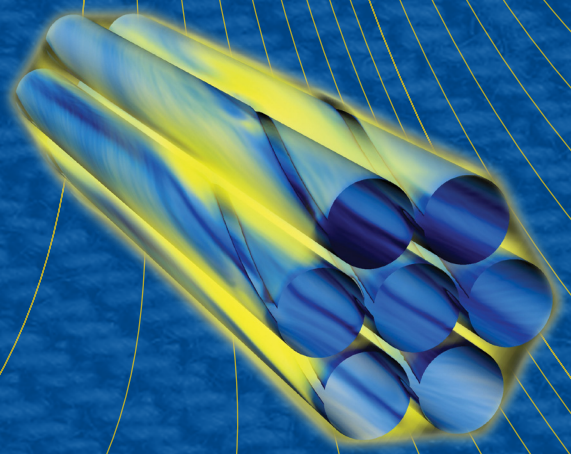


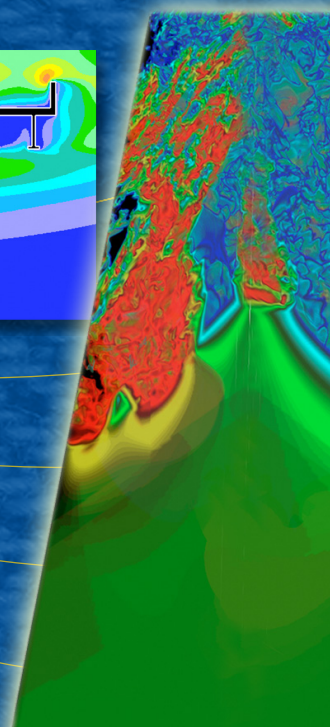












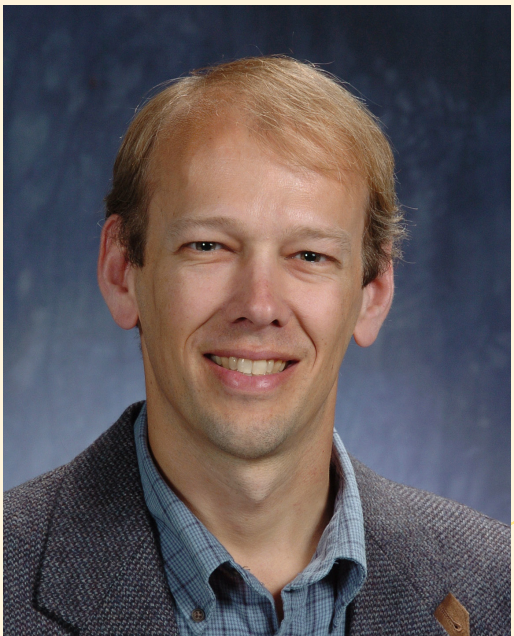
WELCOME

# ARGONNE LEADERSHIP COMPUTING FACILITY

## Dedicated to Breakthrough Science and Engineering

For centuries, scientists have built instruments to aid our understanding of our complex universe. From Galileo's telescope to today's particle accelerators, these devices, combined with our indomitable curiosity to unravel how everything works, have been critical to scientific discovery. It is therefore with great pride that we highlight here a collection of the research projects using one of the newest devices to aid discovery, the supercomputer named Intrepid at the Argonne Leadership Computing Facility.

Sponsored by the U.S. Department of Energy's Office of Science, the Argonne Leadership Computing Facility works hand in hand with the world's best computational scientists to support research in over a dozen different scientific domains, ranging from chemistry, astrophysics, and climate research to computational proteomics and life sciences. This broad range of disciplines also covers a mind-boggling range of physical scales. At one end of the scale, scientists using Intrepid are seeking to understand the interactions of the smallest components in the universe, quarks and gluons, which account for most of the visible matter in the universe. At the other end of the scale, computational scientists are using Intrepid to understand the brightest and most powerful exploding stars. However, scientific discovery with Intrepid is not limited to the hard-to-imagine realms of sub-atomic particles or galaxies light years away. Researchers are using the Argonne Leadership Computing Facility to study and explore key scientific problems that underlie important challenges that face our society. For example, a team of researchers funded by the National Institutes of Health is investigating one of the leading causes of death in the United States: catastrophic rhythm disorders of the heart. Their discoveries could lead to safer and more effective treatment of patients. Likewise, scientists from Pratt & Whitney are using Intrepid to understand the complex processes within aircraft engines. Expanding our understanding of jet engine combustors is the secret to improved fuel efficiency and reduced emissions. Lessons learned from the scientific simulations of jet engine combustors have already led Pratt & Whitney to newer designs with unprecedented reductions in emissions, noise, and cost of ownership.



*Dr. Peter Beckman*
*Division Director, ALCF*

In addition to working with scientists running experiments on Intrepid, we have become a nexus for the broader global community. In partnership with the Mathematics and Computer Science Division at Argonne National Laboratory, we have created an environment where the world's most challenging computational science problems can be addressed. Our expertise in high-end scientific computing enables us to provide guidance for applications that are transitioning to petascale as well as to produce software that facilitates their development, such as the MPICH library, which provides a portable and efficient implementation of the MPI standard – the prevalent programming model for large-scale scientific applications – and the PETSc toolkit that provides a programming paradigm that eases the development of many scientific applications on high-end computers.

Finally, I would like to thank our user community, whose achievements we are showcasing here. They are our most important partners as we boldly seek to solve the world's most challenging and important computational science problems of today and advance toward exascale computational science.

# Providing a Gateway for Scientific Discovery

The Argonne Leadership Computing Facility (ALCF) provides the computational science community with a world-leading computing capability dedicated to breakthrough science and engineering. The ALCF houses the IBM Blue Gene/P system named Intrepid, which debuted in June as the world's fastest computer for open science and third fastest overall. Both rankings represented the first time an Argonne-based supercomputing system placed in the top five of the industry's definitive list of supercomputers.


A gateway for scientific discovery, the ALCF is a U.S. Department of Energy (DOE) national leadership-class computing facility sponsored by DOE's Office of Science. DOE selects major ALCF projects through the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program. This program seeks computationally intensive, large-scale research projects that can make high-impact scientific advances through the use of a large allocation of computer time, resources, and data storage.

In 2008, DOE awarded 20 research projects more than 111 million processor hours of computing time on the Blue Gene/P at the ALCF. The breakthrough science being conducted spans a diverse range of scientific areas—from studying exploding stars to designing more efficient jet engines to exploring the molecular basis of Parkinson's disease. A number of these remarkable research endeavors are highlighted in the following pages.

ALCF staff members provide in-depth expertise and assistance in using the BG/P and optimizing user applications. Both the Catalyst and Applications Performance Engineering and Data Analytics (APEDA) teams support the users' projects.

The Catalyst team establishes strategic collaborations with the ALCF's leading project partners to maximize benefits from the use of ALCF resources. The team provides full project lifecycle assistance, value-added services, and support in conjunction with ALCF hardware and software resources, tailored services for unique requirements of a given research initiative, and close contact with research teams through ongoing interactions with an assigned ALCF project coordinator.

The APEDA team helps ALCF users achieve the best performance in their applications. To this end, team members work closely with users in porting, tuning, and parallelizing their applications on the Blue Gene/P. They also address I/O and data analytics issues that inhibit performance. The team is comprised of staff with extensive experience in computer architectures; computational algorithms; porting, performance tuning, and parallelizing of scientific applications and other software; I/O; and graphics.

## Blue Gene/P Resources

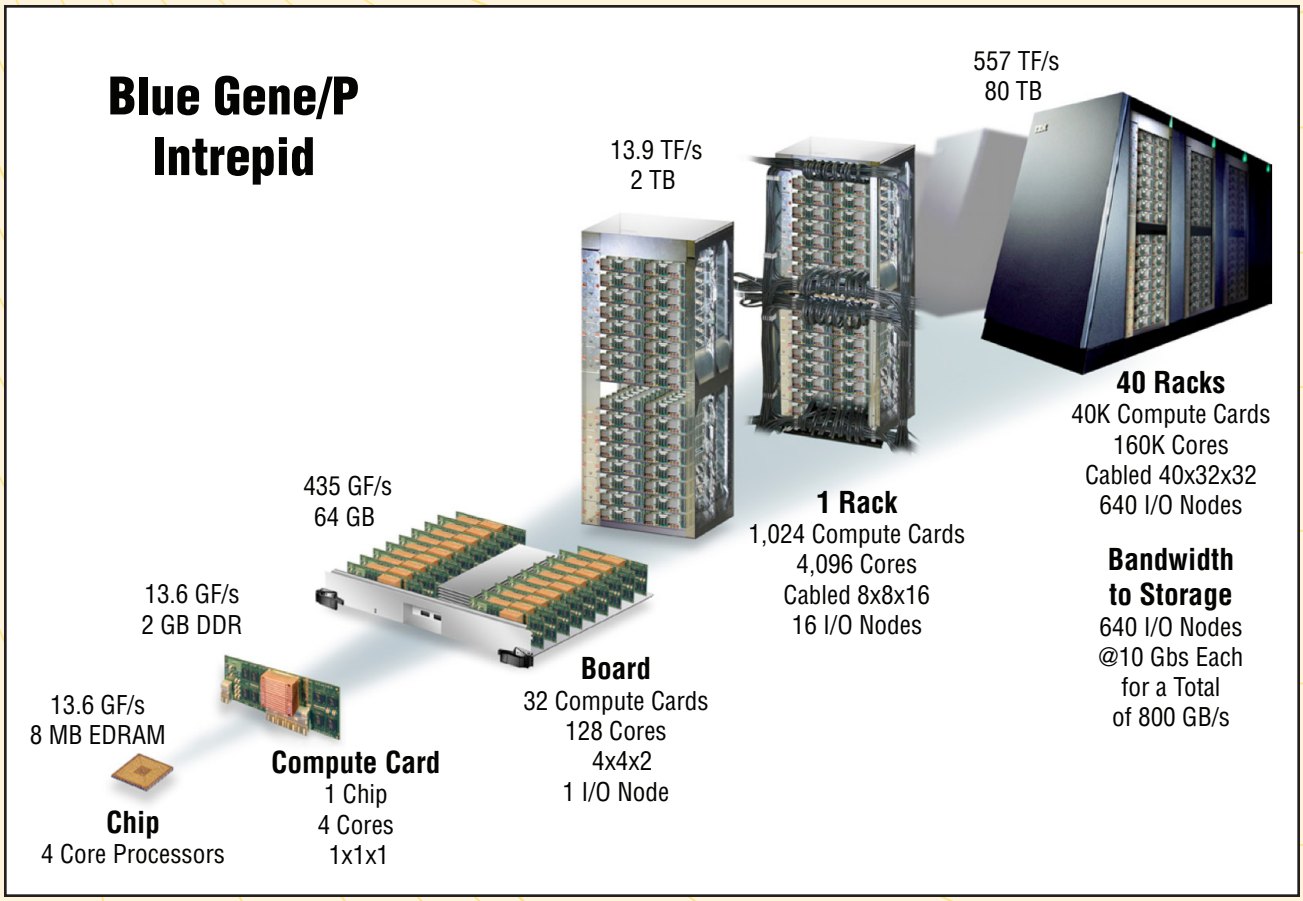
Intrepid is an IBM Blue Gene/P system with a peak speed of 557 Teraflops and a Linpack speed of 450 Teraflops. Intrepid's configuration features 40,960 nodes, each with four processors or cores for a total of 163,840 cores and 80 terabytes of memory.

In 2008, one-fifth of the system is in production. In 2009, the full system will be in production mode, and Intrepid will provide 500 million core hours to INCITE and the high performance computing community.

Currently, part of the system is in Early Science mode, with large-scale applications running most of the time, but some time is dedicated to integrating high-speed I/O systems, extensive online data storage, and an automated tape archive.

For most applications, effective use of such a powerful system requires being able to get high volumes of data in and out quickly and to store large quantities online. Intrepid's data systems consist of 640 I/O nodes that connect to 16 storage area networks (SANs) that control 7,680 disk drives with a total capacity of over 6 petabytes and an aggregate transfer speed of 80 gigabytes per second. Two parallel file systems—PVFS and GPFS–manage the storage. An HPSS automated tape storage system provides archival storage.

The ALCF also operates Surveyor, a BG/P system with 1,024 quad-core nodes (4,096 processors) and 2 terabytes of memory. Surveyor is used for tool and application porting, software testing and optimization, and systems software development.



# Illuminating Scientists' Knowledge of the Universe with "Standard Candles"

Researchers are studying critical aspects of Type Ia supernovae, among the brightest and most powerful exploding stars in the universe. Type Ia create many of the elements from which we are made and are important for measuring distances in the universe.

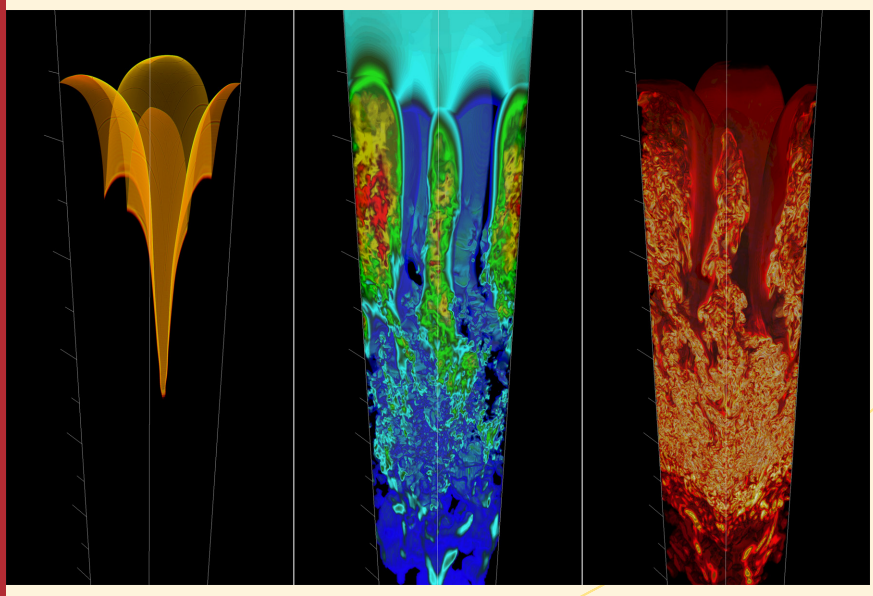
Observations using Type Ia as "standard candles" revealed that the expansion rate of the universe is accelerating and led to the discovery of dark energy. Understanding dark energy ranks among the most compelling problems in all of physical science. Most scientists believe that using Type Ia to determine the properties of dark energy will require accurate simulations of Type Ia and quantification of the uncertainties in the predictions made by these simulations.

Two major challenges facing Type Ia supernova exist:

- Buoyancy-driven turbulent nuclear burning, which is a key physical process in Type Ia, is not fully understood; and
- Few simulations of the four current models of Type Ia have been done, making it difficult to determine which of these models is favored by observations, and even more, what values of the many parameters specifying these models are consistent with observations.

## Approach

Researchers are using computational resources available through the U.S. Department of Energy's INCITE program to meet both of these challenges. Using the FLASH code on Intrepid, the IBM BG/P supercomputer at the Argonne Leadership Computing Facility (ALCF), they are seeking definitive answers to the questions: "Is buoyancy-driven turbulent nuclear burning due primarily to large-scale or small-scale features of the flame surface?" and "At what physical conditions does turbulence tear apart the flame?" In carrying out these two studies, they will build on their success in conducting the largest homogeneous, isotropic, weakly compressible turbulence simulation done to date.



*Images from a large, 3-D, multi-scale, multi-physics simulation of buoyancy-driven turbulent nuclear combustion carried out on the Intrepid supercomputer at the Argonne Leadership Computing Facility. The three frames show different physical properties of the reactive flow, which provide different insights into its nature. The images were produced by the Futures Lab at Argonne National Laboratory.*

## Results/Accomplishments

The results of these two studies have the potential to produce a major paradigm shift in the Type Ia field. The results of the first study will eliminate one of the largest uncertainties in simulating Type Ia. The results of the second study will determine whether the transition from the flamelet burning regime to the distributed burning regime can take place in Type Ia with profound implications for two of the four current Type Ia models.

Working together, the Flash Center and ALCF staff have optimized the FLASH code to run efficiently on all 163,840 processors of the IBM BG/P supercomputer at the ALCF for the buoyancy-driven turbulent nuclear burning simulations. To date, the team has used 40 million processor hours on the BG/P to run a grid of simulations for different physical conditions. They have also developed parallel processing tools needed to analyze the large amounts of data produced by the FLASH simulations of buoyancy-driven turbulent nuclear burning. Preliminary analysis of these results shows that the flame surface is complex at large scales and smooth at small scales.

## Future Efforts

Conducting the larger and more complex simulations needed to determine the physical conditions at which turbulence tears apart the flame will be the next step. The results of both studies will be used to treat buoyancy-driven turbulent nuclear burning more accurately in the Flash Center's whole-star, three-dimensional simulations of Type Ia.

*A study in buoyancy-driven turbulent nuclear burning in Type Ia supernovae. Type Ia supernovae are used as standard candles in the universe and are responsible for many critical discoveries about the structure of the cosmos. Graphics courtesy of the NNSA ASC/Alliance Flash Center at The University of Chicago from research results computed in part at the Argonne Leadership Computing Facility.*

*"Buoyancy-driven turbulent nuclear burning is a key physical process in Type Ia, but we do not fully understand it. The computational resources awarded to the FLASH Center under the INCITE program allow us to carry out large, three-dimensional, multi-scale, multi-physics simulations to determine the nature of this process."*

Donald Lamb, The University of Chicago

**Blue Gene/P Allocation Hours at Argonne: 21,000,000**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# Enabling Breakthrough Innovation at P&G

Some of the world's most well-known and highly regarded industrial companies have sought out Argonne's computing capability and technical expertise to convert that knowledge into transformative products and technologies. Procter & Gamble (P&G), one of the 25 largest U.S. companies by revenue, is among them.

## Approach

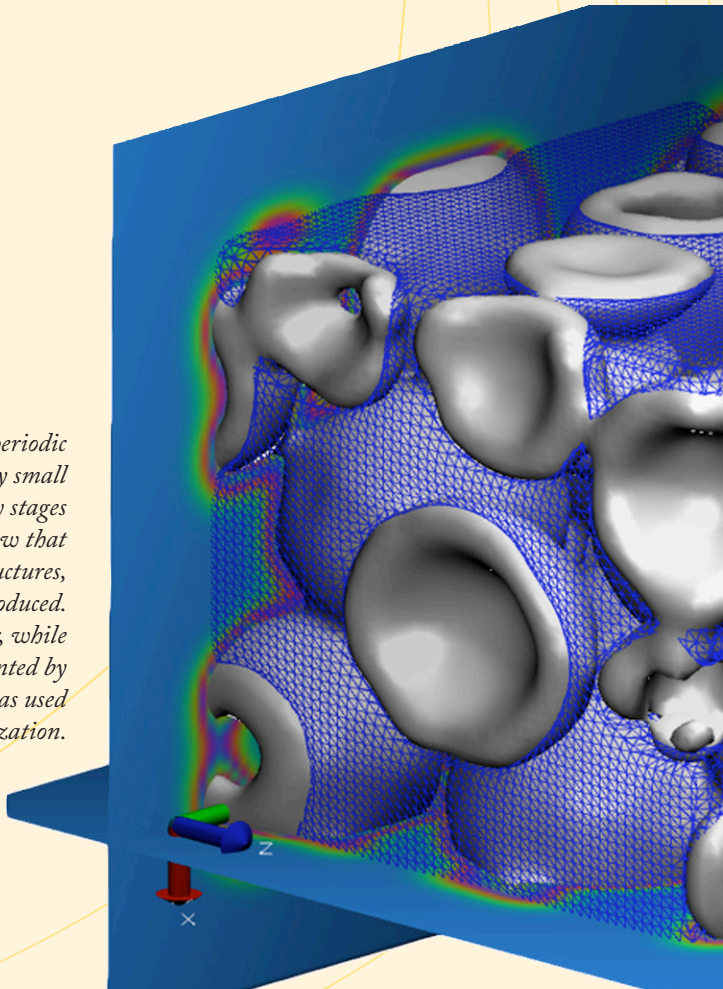
P&G researchers are using the Blue Gene/P system at the Argonne Leadership Computing Facility to investigate the molecular mechanisms of bubble formation in foams. Until recently, most knowledge of how suds form and break down was based primarily on experience and observation. However, an understanding of these processes is critical in the development of many consumer goods, foods, and fire control materials. INCITE allocations from the U.S. Department of Energy allow the researchers to perform computer simulations at an unprecedented scale on the dissolving of soap and forming of suds.

## Results/Accomplishments

To date, researchers have developed coarse-grained models for two relevant surfactants. Ultimately, this work is expected to help P&G formulate products faster and more efficiently. That means the consumer wins by getting better products sooner, and at better value, than would have been possible using traditional methods.

## Future Efforts

Researchers are currently applying multiscale modeling methods to understand the solution and interfacial behavior of foaming molecule mixtures. They are continuing their collaboration with the University of Pennsylvania to advance simulation methods and material understanding.

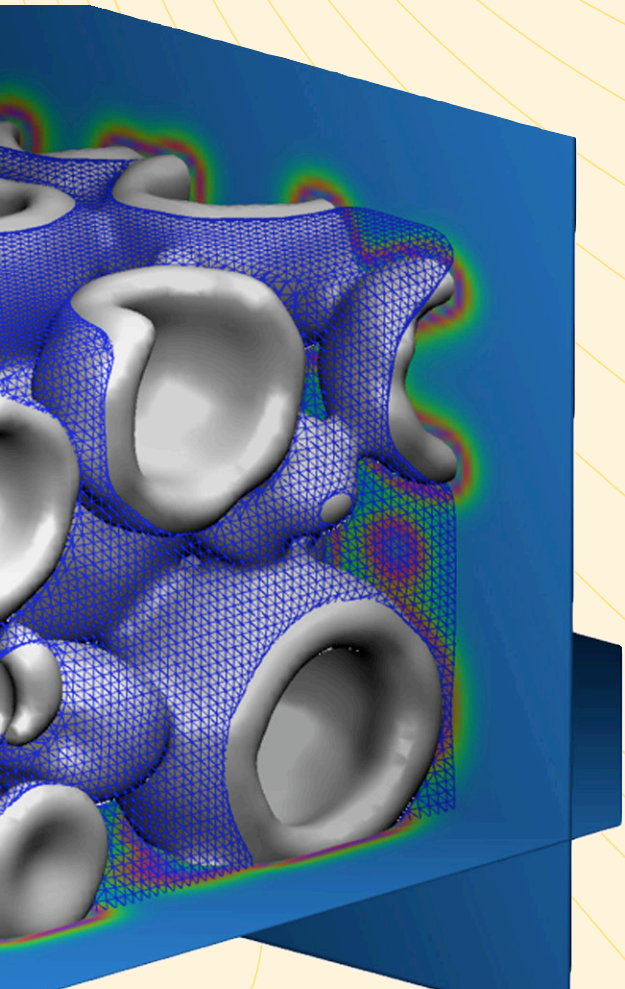



*This image represents a 3-D periodic mesoscale simulation of many small bubbles that exist during the early stages of foam formation. Results show that by using different surfactant structures, different bubble profiles can be produced. The blue mesh represents water, while surfactant molecules are represented by the white isosurfaces. VMD was used to create this visualization.*

*"We wouldn't be able to conduct a computational experiment of this size without our partnership with Argonne. Already through this research, we have experienced a dramatically exciting new approach to evaluate materials. Fully matured, these methods could be used, for example, to evaluate bio-based replacements for petroleum-based ingredients—even guiding their development more effectively. Clearly, these learnings can be applied at P&G, but also extended to other wide-ranging uses outside the company, including formulations for other foam-based materials—even fire control chemicals."*

Tom Lange, Procter & Gamble

**Blue Gene/P Allocation Hours at Argonne: 4,000,000**




Contact:

Kelly Anderson
Procter & Gamble
anderson.kl.1@pg.com

# Improving Aircraft Engine Combustor Simulations

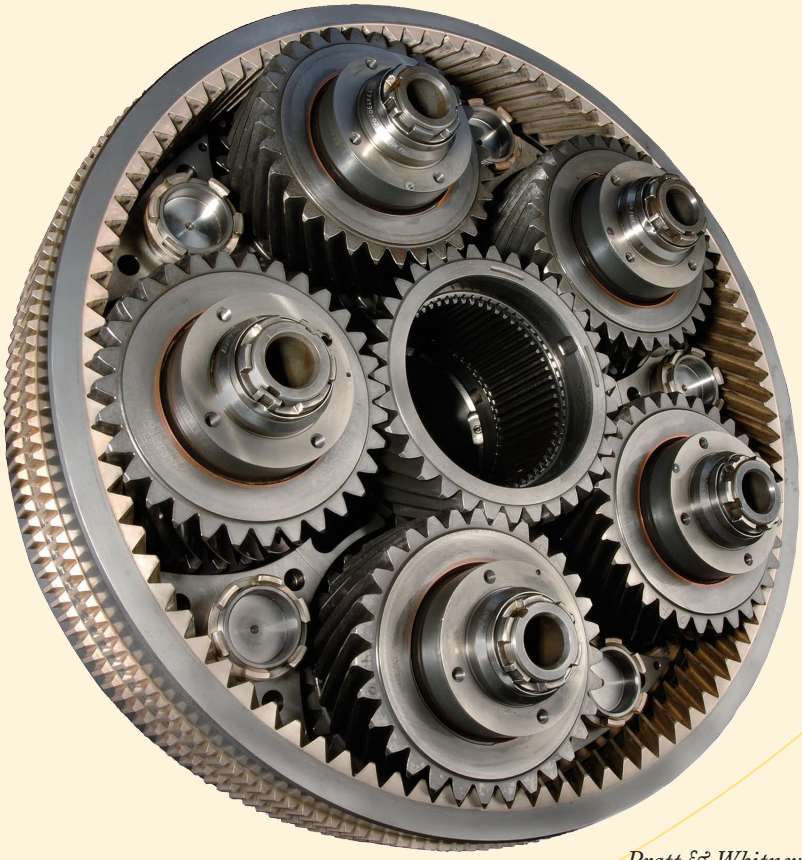
A jet engine combustor combines air flowing faster than a hurricane with swirling fuel to generate the extraordinary release of heat that ultimately powers the aircraft. Understanding these complex physical and chemical interactions is critical to fuel efficiency and emissions performance, but physical testing can be difficult and time consuming.

## Approach

Computer simulation of the complex physics of a combustor creates a "virtual test," thus reducing the need for physical testing. Pratt & Whitney has been exploring leading-edge combustor design methods using the Blue Gene/P supercomputer at the Argonne Leadership Computing Facility as part of DOE's INCITE program.

## Results/Accomplishments

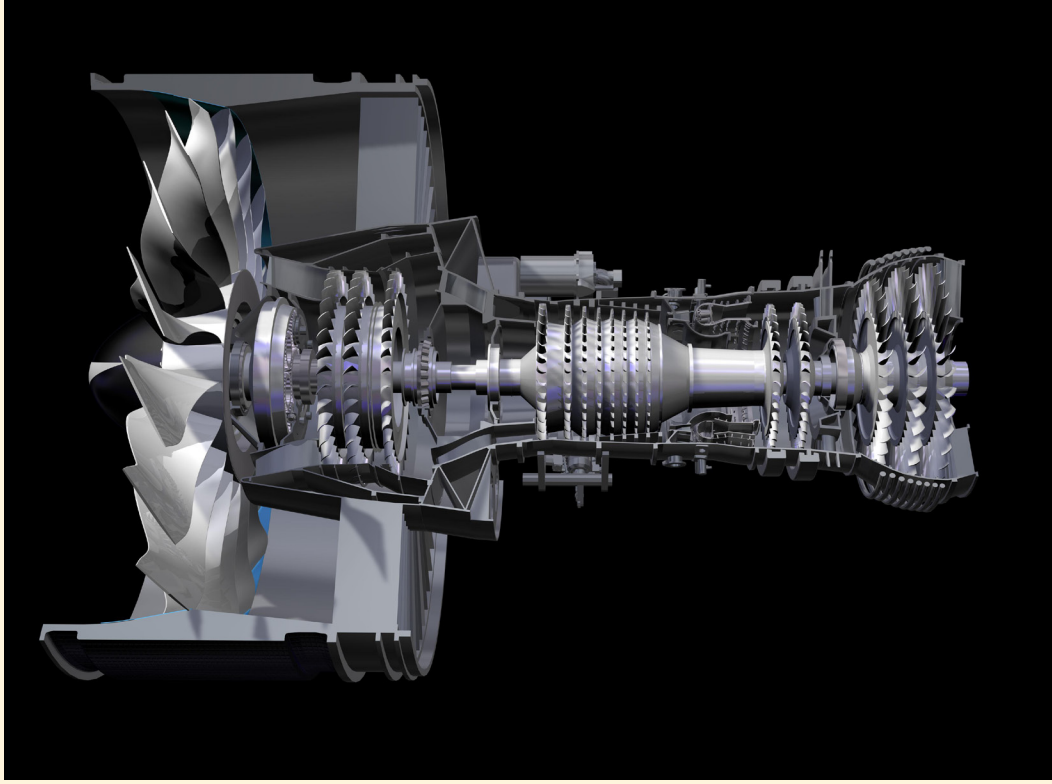
This INCITE project has led to improved capabilities and reduced solution times for 3-D combustor simulations. The work has been a key enabler for the depth of understanding needed to meet emissions goals. INCITE 2006-2007 technologies are now being applied to Pratt & Whitney's next-generation, low-emission Geared Turbofan™ engine. This groundbreaking engine will deliver unprecedented reductions in emissions, noise, and cost of ownership compared to current engines.



*Pratt & Whitney is exploring leading-edge jet engine combustor design methods using the ALCF's Blue Gene/P.*

## Future Efforts

Researchers plan to use the Blue Gene/P to complete high-fidelity simulations that will give new insights on aerodynamic behavior inside an operating jet engine combustor.



*The Geared Turbofan™ engine will deliver game-changing performance, including double-digit improvements in fuel burn and environmental emissions.*

*"In an ever-expanding global economy where technology leadership is critical to competitiveness, INCITE provides American industry with an engine for technological and competitive growth."*

Pete Bradley, Pratt & Whitney

**Blue Gene/P Allocation Hours at Argonne: 1,377,000**


Contact:

Pete Bradley
Pratt & Whitney
peter.c.bradley@pw.utc.com

# Breaking New Ground in Membrane Protein Research

Many biological processes are controlled by proteins in the cell membrane, ranging from production of biofuels to cleaning up toxic organic waste. Large-scale gating motions, occurring on a relatively slow time scale, are essential for the function of many important membrane proteins such as transporters and channels. Voltage-activated ion channels are literally electric switches that are turned "on" by a change in the cellular potential. Malfunction of those channels can lead to cardiac arrhythmia and neurological pathologies.

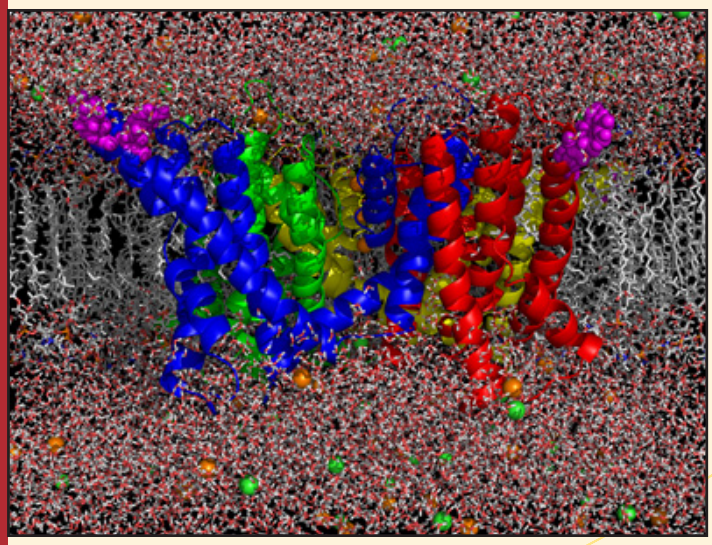
Researchers are modeling the molecular function of a voltage-gated potassium ion channel at leadership-class facilities at Argonne National Laboratory and Oak Ridge National Laboratory (ORNL). The long-term goal of this study is to understand how the membrane-associated molecular protein-machines are able to carry out their functions.

## Approach

A research team from Argonne, The University of Chicago, the University of Illinois at Chicago, and the University of Wisconsin used high-performance computing to break new ground in understanding how these membrane proteins work. Exploiting state-of-the-art developments in molecular dynamics and protein modeling, the team constructed models of voltage-gated potassium channels and ran them on Argonne's Blue Gene/P and ORNL's CRAY XT leadership-class computers, using U.S. Department of Energy INCITE resources.

## Results/Accomplishments

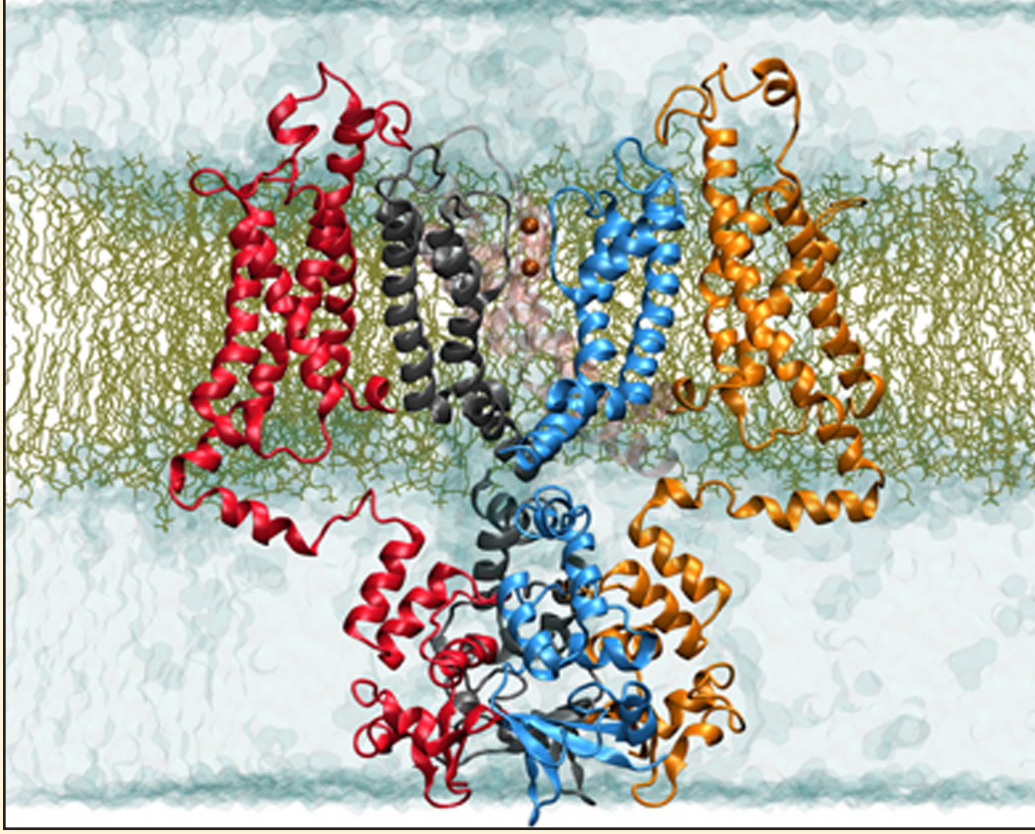
An important result of these simulations concerns the properties of the electric field responsible for the voltage activation. The calculations show that this electric field is indeed more intense than at other equivalent positions across the membrane far away from the protein. These results from simulations open up the possibility of better-designed therapeutic drugs, as well as the construction of artificial biomemetic nano-switches.



*Atomic model for the simulation of the KvAP channel in a lipid membrane. The model represents the channel in an open activated state as determined by EPR experiments from the laboratory of Eduardo Perozo (The University of Chicago). The atomic model comprises 964 amino acids, 302 lipid molecules, 12,046 water molecules, and 53 $K^+$ and $Cl^-$ ion pairs. In total, there are 112,798 atoms in the system. The positively charged arginine residues of the voltage sensors are colored in magenta. The simulations of about 50 ns were performed by using the NAMD package with up to 512 processors on the BG/L at the Argonne Leadership Computing Facility.*

## Future Efforts

The next challenge to be addressed will be the conformational pathway for the open and closed gating transition of the channel. Advanced and novel strategies will be essential in determining the reaction pathway and the interconversion rate by describing the transition process through a chain of states.



*Complete model of the Kv1.2 channel assembled using the Rosetta method. The atomic model comprises 1,560 amino acids, 645 lipid molecules, 80,850 water molecules, and ~300 $K^+$ and $Cl^-$ ion pairs. In total, there are more than 350,000 atoms in the system. The simulations were generated by using NAMD on the Cray X-T (Jaguar) at Oak Ridge National Laboratory and the BG/P at the Argonne Leadership Computing Facility.*

*"Being able to run on these top computers is essential for this work. The time and energy scales of the underlying molecular processes are just within reach of the computational capabilities of such leadership-class computers."*

Benoit Roux, Argonne National Laboratory and The University of Chicago

**Blue Gene/P Allocation Hours at Argonne: 1,500,000**
**Jaguar Allocation Hours at ORNL: 3,500,000**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Argonne National Laboratory and The University of Chicago
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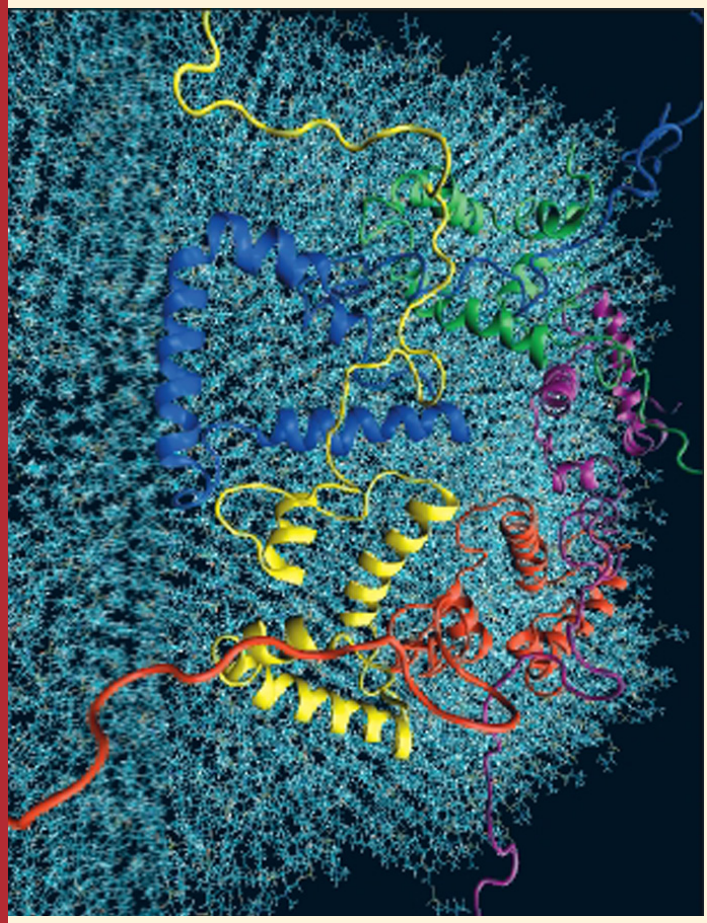
# Modeling the Molecular Basis of Parkinson's Disease

As the second most common neurological disorder in adults, the personal and economic impacts of Parkinson's disease are enormous. Every nine minutes, an individual is diagnosed with the disease. Currently, there are more than 2 million cases in the United States, with 60,000 new cases diagnosed each year. In economic terms, the disease exacts an annual cost of $25 billion on the U.S. economy alone.



*Alpha-synuclein pentamer constructed with 4ns molecular dynamics (MD) conformers after equilibration on the membrane with MD.*

## Approach

Researchers are leveraging the power of the Blue Gene/P at the Argonne Leadership Computing Facility to learn more about the molecular basis of the disease and explore ways to treat it. Using molecular models and simulations together with biochemical and ultrastructural analysis, University of California—San Diego scientists have shown that the clumping of a protein known as alpha-synuclein (aS) in the brain can lead to harmful, pore-like structures in human membranes. In contrast, another protein, beta-synuclein (bS), appeared to block the clumping action. Allocations from the U.S. Department of Energy INCITE program have made this approach possible.

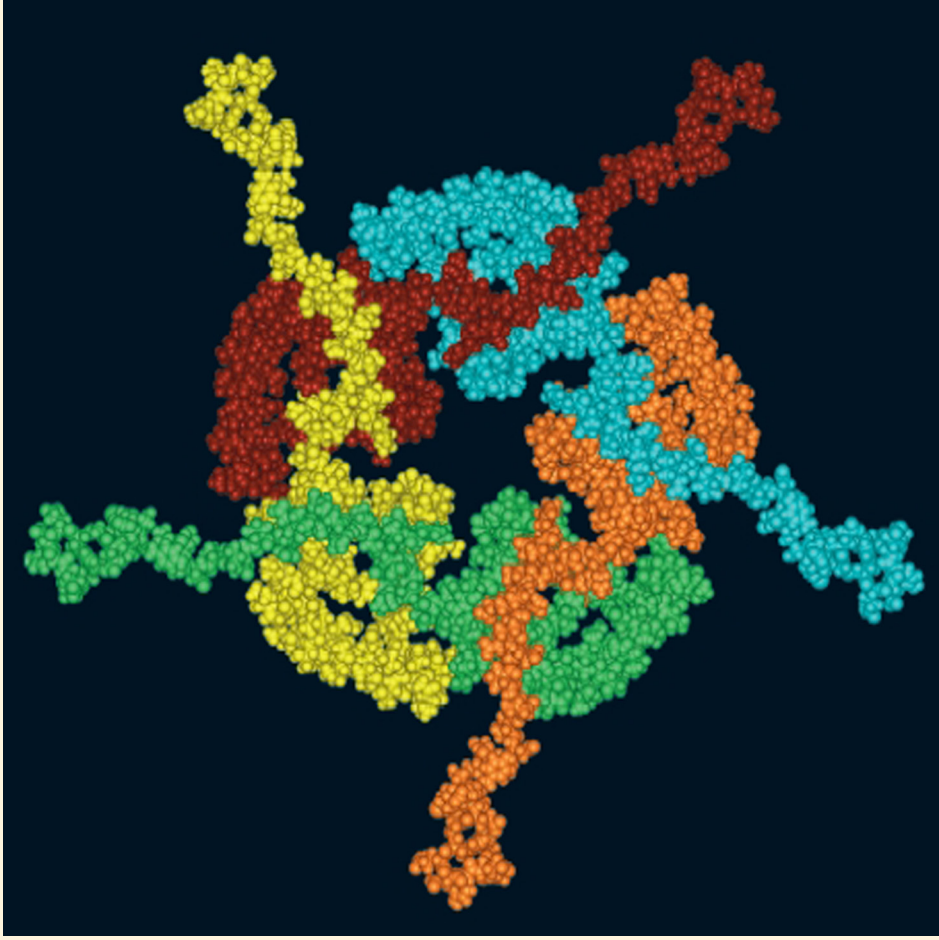
## Results/Accomplishments

The research is providing insights into the molecular mechanism for Parkinson's disease progression and will have broad applicability to other diseases. The findings also provide a test bed for identifying possible therapeutic interventions through computational modeling. Given the encouraging correlation between the molecular dynamics modeling predictions and laboratory experimental results, the team expects to make steady progress with the computational model for Parkinson's disease progression and design of effective drugs based on the computational modeling and simulations.

**Blue Gene/P Allocation Hours at Argonne: 1,200,000**

## Future Efforts

The research team will focus on a more comprehensive investigation of alpha-synuclein penetration into the membrane, including a thorough study of pore creation. The scope of the team's work has increased in both the number of simulations being conducted and the scale of the simulations.



*Consecutive docking of a membrane-philic conformation of alpha-synuclein monomers on the membrane leads to the creation of a pentameric ring structure.*

*"The anti-Parkinson's drug based on the results of our modeling and simulations is in the early stages of development. The intermediate pro-drug showed preliminary results of slowing aggregation of alpha-synuclein—the unstructured protein that has been shown as one of the main causes of Parkinson's disease. These studies are impossible without a high-performance computer, which is the Blue Gene at Argonne National Laboratory."*

Igor Tsigelny, University of California—San Diego/SDSC

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# Preventing Cardiac Rhythm Disorders

Catastrophic rhythm disturbances of the heart are a leading cause of death in the United States. Treatment and prevention of cardiac rhythm disorders remain difficult because the electrical signal that controls the heart's rhythm is determined by complex, multi-scale biological processes. However, recent advances in experimental technologies have allowed for more detailed characterizations of normal and abnormal cardiac electrical activity.

## Approach

In work funded by the National Institutes of Health (NIH), researchers are using U.S. Department of Energy INCITE allocations on the ALCF's Blue Gene/P to rapidly test hypotheses for the initiation and maintenance of rhythm disorders. These large-scale computer simulations represent a promising tool to help identify the underlying electrical mechanisms for dangerous arrhythmias and determine the effects of interventions, such as drugs, that may prevent or exacerbate these arrhythmias.

## Results/Accomplishments

The results of these simulations may help elucidate mechanisms of heart rhythm disorders that pose a significant health risk to the general public. An improved understanding of these disorders will help lead to safer and better treatments for patients.

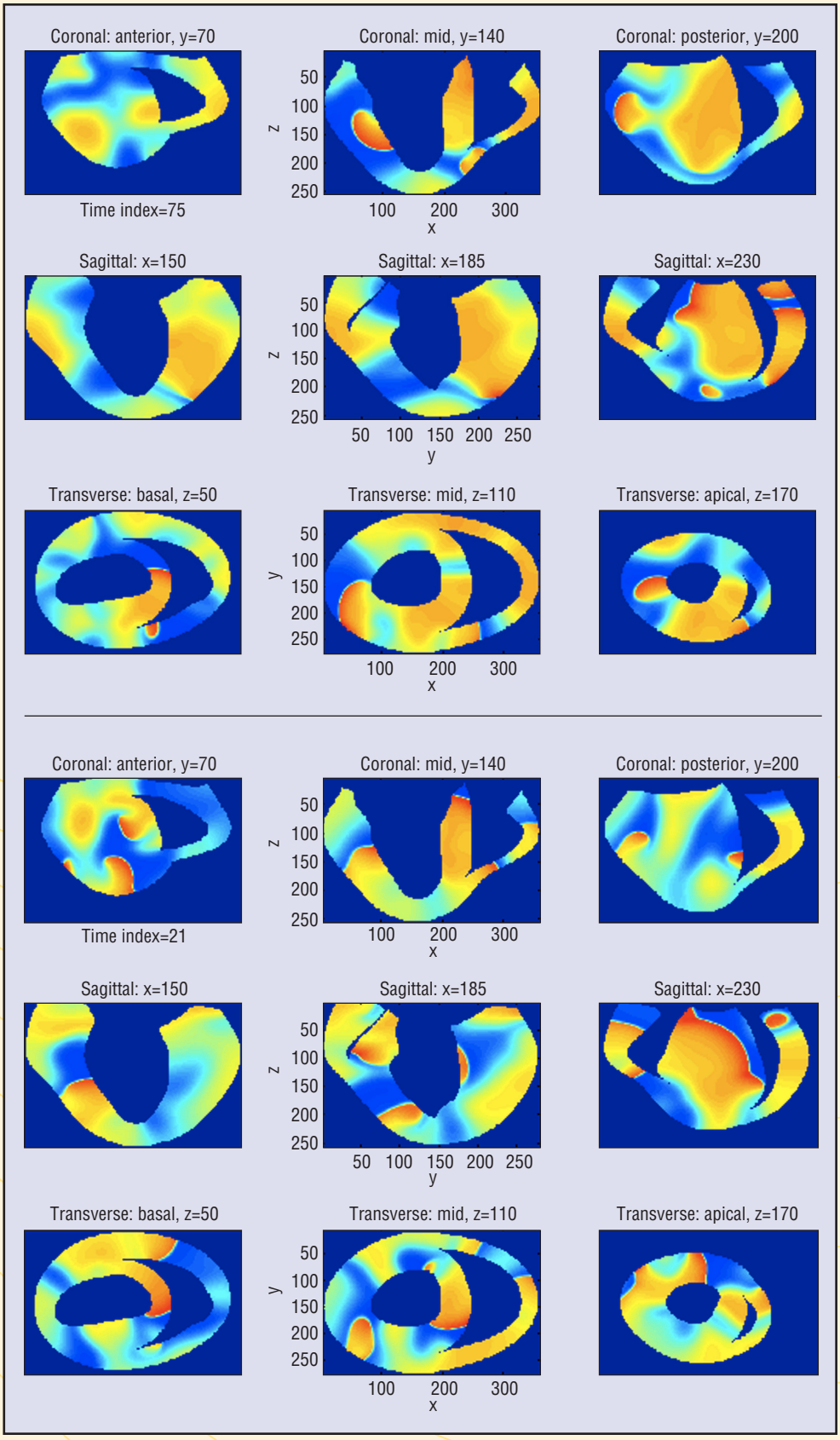
## Future Efforts

Certain activation sequences have been shown to be particularly effective at inducing arrhythmias in canine experimental models. We plan to study these sequences in large-scale simulations of the canine heart to identify the mechanism by which wave break and the induction of an arrhythmia might occur.

*"We're excited about the INCITE award and the opportunity to use the Argonne machine. It will help us conduct large-scale simulations that we could not consider attempting without such a resource."*

Jeff Fox, Gene Network Sciences

**Blue Gene/P Hours Allocated at Argonne: 846,720**




*Simulation of ventricular fibrillation (VF), a dangerous cardiac rhythm disorder, in a three-dimensional model of the canine ventricular anatomy. The panels show two-dimensional cross-sections of electrical activity (red corresponds to excited tissue, and blue to tissue at resting potential). Three cross-sectional planes are shown for each of three orientations: coronal (top), sagittal (middle), and transverse (bottom). Disorganized patterns of electrical activation during VF prevent the heart from contracting properly, causing a potentially fatal disruption of blood circulation. The simulation was conducted on the Blue Gene/P machine at Argonne.*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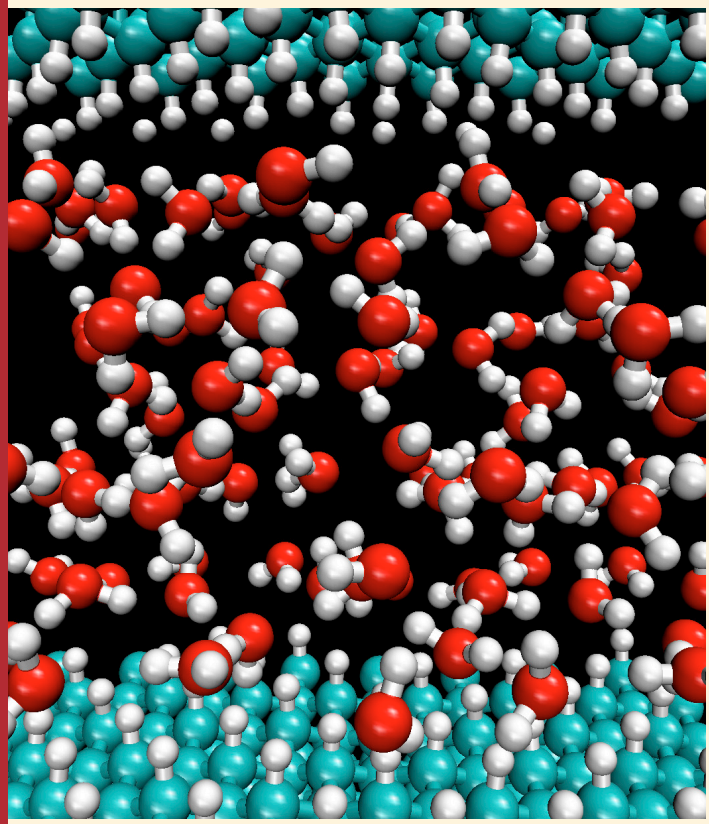
# Probing the Properties of Water

Unraveling the properties of water at organic and inorganic interfaces is a key step towards understanding the function of biological systems and the behavior of soft and hard materials in many natural environments. Probing such properties is a very challenging task, both from an experimental and theoretical standpoint. The challenge is even greater if water is confined in very small spaces—within a few nanometers—as is the case, for example, close to the surfaces of proteins, in channels devised to transport matter at the nanoscale (nanofluidic devices), or in natural rocks such as zeolites or clays.



*Snapshot of an ab-initio molecular dynamics simulation of water confined between a hydrogenated diamond slab. Oxygen, carbon, and hydrogen atoms are represented as red, green, and white spheres, respectively.*

## Approach

Exploiting the power of IBM Blue Gene supercomputers at the Argonne Leadership Computing Facility and IBM Blue Gene Watson Research Laboratory, a team of researchers is using first-principles simulations to investigate what happens at the microscopic level when water meets hydrophilic and hydrophobic surfaces and how the properties of this ubiquitous liquid are modified at the nanoscale. The findings can be applied to solve complex problems in both biology and materials science.

## Results/Accomplishments

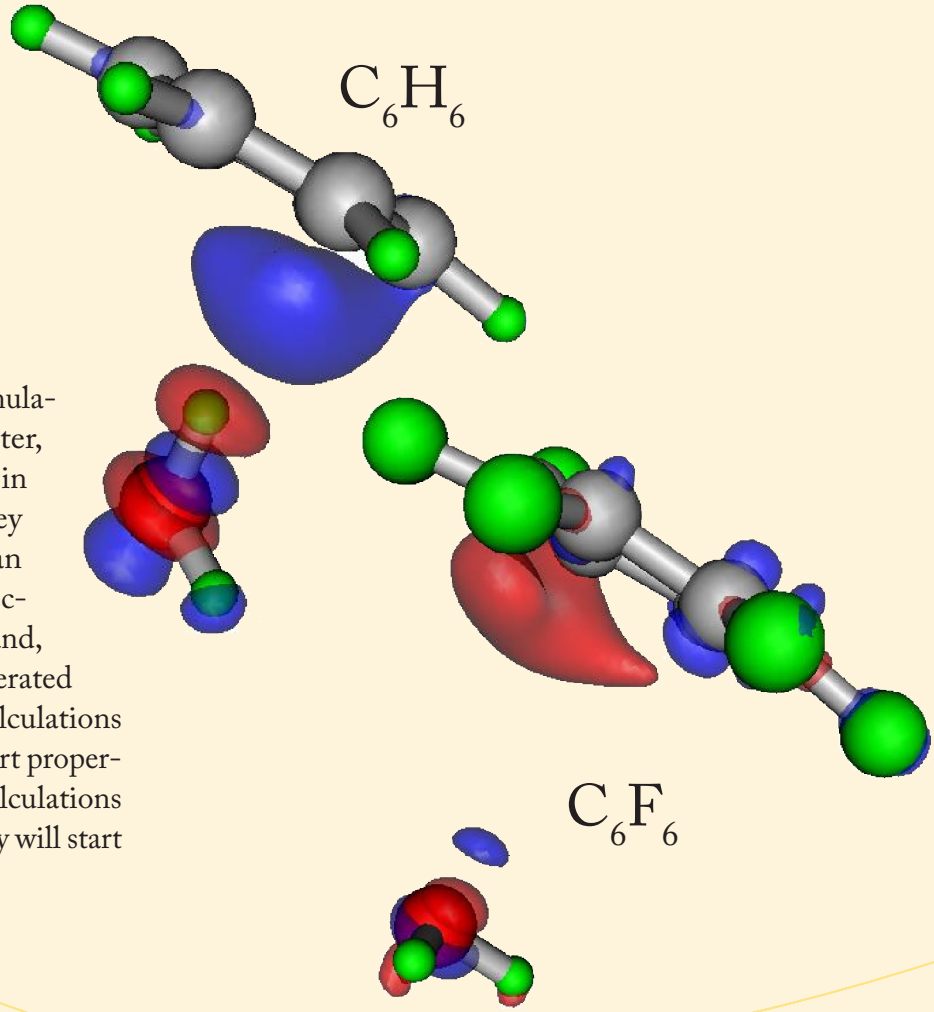
To date, the researchers have studied both pure water and water at interfaces with graphite, nanotubes, hydrogenated diamond surfaces, and biocompatible materials such as silicon carbide.

The first-principles theory used in the team's simulations—density functional theory— yields results that compare well with experiments for all the major structural properties of water, some of its electronic spectroscopic signatures (in a qualitative manner), and several dynamical properties.

In addition, the team identified the key role played by electrons in determining the arrangements of water molecules at the surface. They also computed vibrational spectra and provided predictions and interpretations of what should be seen experimentally when measuring how water molecules vibrate in contact with surfaces.

## Future Efforts

Researchers will complete *ab-initio* simulations of solvated ions in confined water, in particular, alkali and halogens ions in water confined in carbon nanotubes. They also will begin calculations of Raman spectra of water, in addition to IR spectra simulations that have been started and, for some substrates (graphene and deuterated diamond), completed. Electric field calculations will be started as planned. As for transport properties, researchers are testing viscosity calculations using classical potentials, after which they will start *ab-initio* simulations.




*Snapshot of ab-initio molecular dynamic simulations of benzene (top) and hexafluoro-benzene (bottom) in liquid water, showing the electronic charge density (blue and red isosurfaces) and just one water molecule in close proximity with the solute.*

*"It truly is an exciting time for the application of quantum simulations to solving important scientific problems. Key to our success is access to high-performance computing to carry out the large-scale simulations essential to simulations at the nanoscale."*

Giulia Galli, University of California—Davis

**Blue Gene/P Allocation Hours at Argonne: 6,000,000**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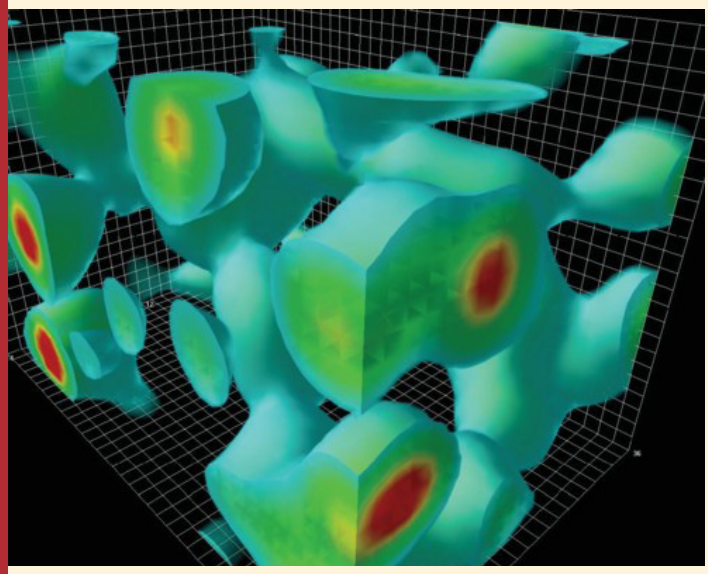
# Deepening the Understanding of Interactions between Quarks and Gluons

This research aims to deepen the understanding of the interactions of quarks and gluons, the basic constituents of 99% of the visible matter in the universe, and will play a key role in ongoing efforts to develop a unified theory of the four fundamental forces of nature.

## Approach

Scientists conducting research in Lattice Quantum Chromodynamics (QCD) have logged more than 100 million core hours on the Blue Gene/P at the Argonne Leadership Computing Facility. The scientists are generating gauge configurations with up, down, and strange quarks on lattices that are sufficiently fine-grained and have sufficiently small up and down quark masses, to enable the extrapolation of key quantities to their physical values found in nature. This work has been made possible through allocations awarded by the U.S. Department of Energy's INCITE program.



*A frame from an animation illustrating the typical four-dimensional structure of gluon-field configurations used in describing the vacuum properties of QCD.*

## Results/Accomplishments

The BG/P has tremendously accelerated the generation of the gauge configurations. In many cases, the rate of progress has been accelerated by a factor of 5 to 10 over what has been possible with other machines. Significant progress has been made in simulations with two different implementations of the quarks–domain wall and staggered.

The domain wall configuration generation is going extremely well, with a statistically meaningful ensemble now available for a lattice size of $32^3 \times 64$. Generation of $48^3 \times 64$ ensembles has also been demonstrated. These are the largest domain wall lattices ever attempted and will be the central focus as soon as more statistics from the smaller ensemble have been obtained. Substantial analysis for K meson physics is under way, and analysis needed to study nucleon structure is starting.

For the staggered quarks, a set of runs with a lattice spacing of 0.06 femtometers (fm) is nearing completion, and a new ensemble with a spacing of 0.045 fm and lattice size of $64^3 \times 192$ is about one-fourth complete. These are the most challenging staggered ensembles generated to date. These configurations are being used to calculate the decay constants of pi and K mesons, the weak transition coupling (CKM matrix element) between the up and strange quarks, and the masses of the lightest strongly interacting particles. This work will greatly improve the accuracy of the research team's determination of all of these quantities and a wide range of other quantities of importance in high energy and nuclear physics.

*"The combination of Early Science Program and INCITE time made available at the ALCF over the past three months has advanced the study of chiral fermions and of improved staggered quarks by nearly a year. We expect to present scaling results for neutral K meson mixing, quark masses, pseudo scalar decay constants, the light hadron spectrum and nucleon form factors at Lattice 2008 in July, which would otherwise have been unavailable until well into 2009."*

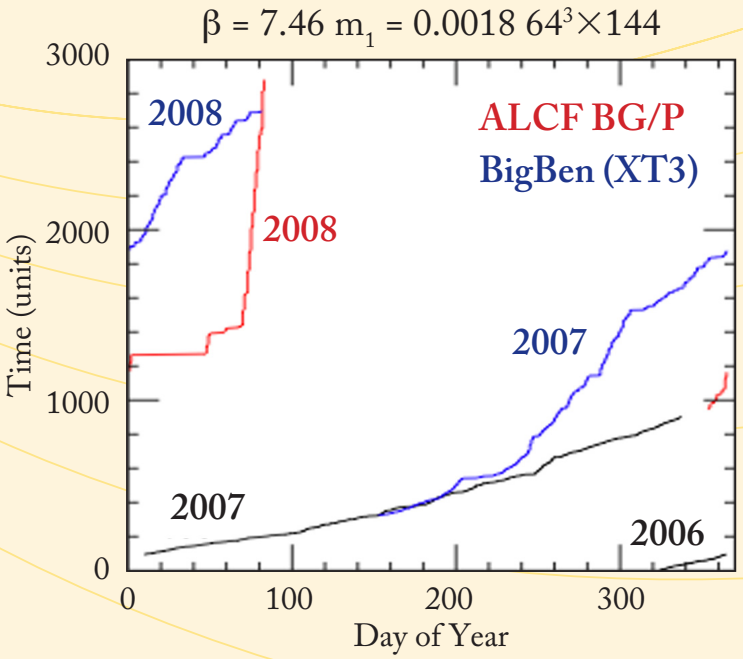
Bob Sugar and Norman Christ, U.S. QCD Consortium

**Blue Gene/P Allocation Hours at Argonne: 19,600,000**

## Future Efforts

A portion of planned future calculations focuses on completing the data sets now being created on the Argonne BG/P. For the domain wall fermion work, researchers must make good on the initial promising experiments begun with a $48^3 \times 64$ lattice volume. This will permit calculation with the lightest quark masses studied to date using chiral fermions, reducing the errors associated with extrapolating to the physical quark masses by perhaps a factor of two. However, the most exciting next steps await the results of the current Argonne running. If early strong indications of large chiral corrections are borne out, the next set of questions in weak interaction and nucleon physics will require substantially larger lattice volumes. The researchers have been working intensely over the past nine months to develop new methods that will permit such studies to be carried out using the Argonne BG/P machines. They expect that production running using these new methods could begin by early fall.

The research team working with staggered quarks is about to use the configurations generated at the ALCF in its studies of the decays and mixings of particles containing heavy quarks, specifically the D, Ds, B, and Bs mesons. These calculations, coupled with recent experimental results, will enable substantial improvements in determining a number of elements of the CKM matrix. The CKM matrix elements are among the least well known parameters of the Standard Model of subatomic physics, which encompasses current understanding of the fundamental forces of nature. The planned calculations will enable precise tests of the Standard Model, aiding in the effort to obtain a deeper understanding of fundamental physics.




*Acceleration in the generation of a = 0.06 fm, $64^3 \times 144$ configurations provided by the BG/P. The black and blue curves are for older supercomputers, and the red the BG/P.*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# Making Safe, Clean Nuclear Energy Available Globally

As part of the nuclear energy program, the United States is committed to new technologies that will dramatically expand the availability of safe, clean nuclear energy to help meet the growing global energy demand. Liquid-metal-cooled fast reactors are a key component of this strategy in that they permit recycling of nuclear fuel and are expected to be economical sources of power.

## Approach

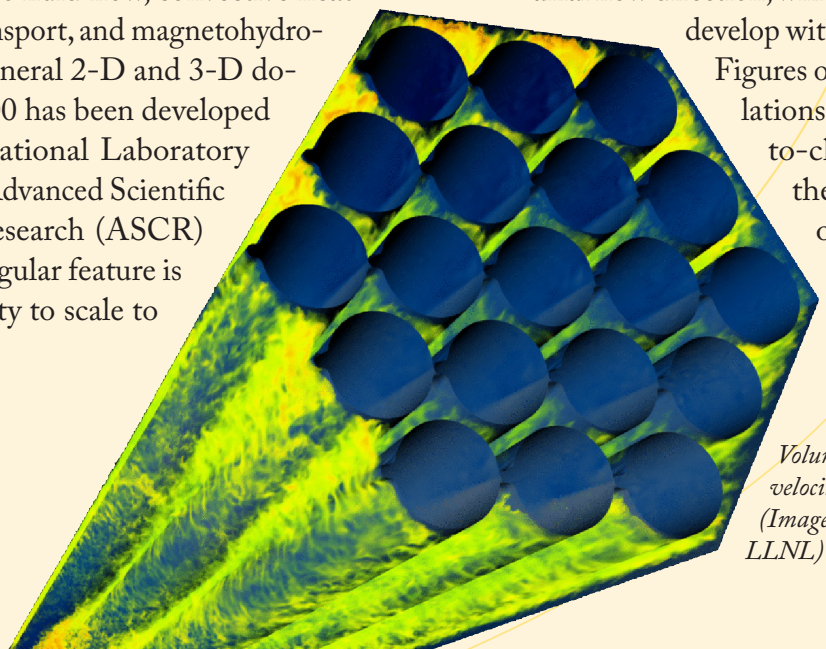
Through U.S. Department of Energy (DOE) INCITE allocations, researchers are carrying out large-scale numerical simulations of turbulent thermal transport in sodium-cooled reactor cores. These simulations will enable researchers to gain an understanding of the fundamental thermal mixing phenomena within advanced recycling reactor cores, which can lead to improved safety and economy of these pivotal designs.

The simulations are running on P=4,096 up to P=32,768 processors of the IBM Blue Gene/P at the Argonne Leadership Computing Facility. The computations are based on the Nek5000 code, which simulates fluid flow, convective heat and species transport, and magnetohydrodynamics in general 2-D and 3-D domains. Nek5000 has been developed at Argonne National Laboratory under DOE's Advanced Scientific Computing Research (ASCR) program. A singular feature is the code's ability to scale to the large processor counts that characterize petascale computing platforms. Nek5000 was recognized with the 1999 Gordon Bell prize for algorithmic quality and sustained high performance on 4,096 processors of the ASCI-Red.

## Results/Accomplishments

Researchers have simulated wire-wrapped fuel rods with 7- and 19-pin bundles. The current computations are some of the largest to date with Nek5000 and involve several hundred million gridpoints in unstructured domains. The scale of these computations has necessitated development of a new parallel strategy for solving the coarse-grid problem that is central to the efficiency of Nek5000's multigrid solvers. The new solver employs algebraic multigrid, using Nek5000's existing communication kernels, and results in sustained parallel efficiencies of ~60% for P=32,768 with only 3,700 points per processor.

The figure below shows a volume rendering of the axial velocity for a 19-pin bundle. To reduce computational costs, the simulations were performed using periodic boundary conditions in the axial flow direction, which allows turbulence to develop within a single wire-pitch. Figures of merit for these simulations include the channel-to-channel mixing and the pressure drop, both of which are significantly influenced by the presence of the



*Volume rendering of axial velocity in a 19-pin bundle. (Image by D. Bremer, LLNL)*

*"Work on high-performance computers, such as the Blue Gene/P, allows us to simulate materials and designs important to the safety and reliability of the nation's nuclear energy resources."*

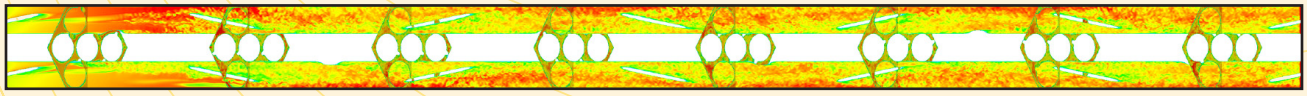
Paul Fischer, Argonne National Laboratory

**Blue Gene/P Allocation Hours at Argonne: 14,000,000**

side channels that are bounded by only two pins and a wall.

The second figure shows the velocity for a 7-pin bundle with three-wire pitches and a laminar inflow condition. This simulation illustrates that the flow becomes fully turbulent within a single wire pitch, which justifies the use of periodic boundary conditions when computing the turbulent flow field over lengths that span several wire pitches and many channel diameters. Calculations of this magnitude would not have been possible without resources at the BG/P scale.

University of Illinois and Argonne teams are working closely together to validate the core hydrodynamics large-eddy simulations by comparing highly detailed simulations in similar configurations. The university partners are performing simulations of coolant flow in a simplified geometry that allows them to resolve all turbulent motion with no modeling assumptions. These results are being compared to the Nek5000 computations, which simulate only the largest turbulent eddies in the flow. The validated Nek5000 results are being used to benchmark steady-state Navier-Stokes codes that employ turbulence models and to provide input to reactor design codes that require only coarse (mean flow) data. Visualization support for this project is being provided by the VisIt group at Lawrence Livermore National Laboratory (LLNL).



*Axial and centerplane plots of axial velocity in a 7-pin bundle: The flow transitions from laminar to turbulent within a single wire pitch as it moves downstream of the inlet (left).*

## Future Efforts

Experiments indicate that low pin count results do not extrapolate to higher pin counts because of the edge channel effects. Succeeding simulations will involve more fuel pins, culminating in the design target of 217 pins. The group will be studying coolant flow in a variety of core subassembly designs in order to optimize reactor performance.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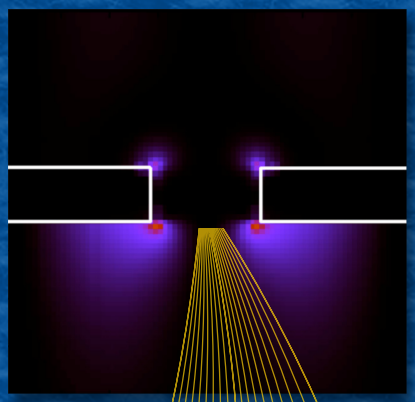

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